

### Aksiomi

- 1) Stanje  $|\psi\rangle$  je element Hilbertovog prostora.  $\langle\psi|\psi\rangle = 1$
- 2) Operacijske so opisane s Hermitovimi operatorji:  $A = A^\dagger$
- 3) Bosnovo pravilo:  $\hat{A} = \sum_{i=1}^n \lambda_i |i\rangle \langle i|$        $\langle i|j\rangle = 0 \text{ & } \lambda_i \neq \lambda_j$   
 ↓  
 lastni vektor  
 lastna rednost

Pri među lastnicima A dobivo rezultat  $\lambda_i + \text{vejetacije} |\langle i|t\rangle|^2$ .

- 4) Među su destruktivne. Če  $A_n$ , potem je sistem točkoj po među u stanju  $|n\rangle$ .
- 5) Časovi potreba opisuje učna unutarna matrica,  $U U^\dagger = I = U^\dagger U$ .

### Schrödingerova enačba

$$|\psi(t_2)\rangle = U(t_2, t_1) |\psi(t_1)\rangle \quad |\psi(t_2)\rangle = U(t_3, t_2) |\psi(t_2)\rangle$$

$$\begin{aligned} |\psi(t_3)\rangle &= U(t_3, t_2) |\psi(t_2)\rangle = U(t_3, t_1) U(t_2, t_1) |\psi(t_1)\rangle \\ &= U(t_3, t_1) |\psi(t_1)\rangle \end{aligned}$$

$$U(t_3, t_1) = U(t_3, t_2) U(t_2, t_1) \quad t_3 \geq t_2 \geq t_1$$

$$U(t+\Delta t, t) \rightarrow |\psi(t+\Delta t)\rangle = U(t, \Delta t) |\psi(t)\rangle$$

$$\Delta t \rightarrow 0 \quad U(t, t) = I \quad \hat{U}(t+\Delta t, t) = I + \Delta t \hat{K}$$

$$U \rightarrow U_{ij} = \langle i| \hat{U}|j\rangle \quad U_{ij}(t+\Delta t, t) = \delta_{ij} + \Delta t K_{ij}$$

$$U^\dagger U = I \rightarrow \sum_i (U^\dagger)_{ij} U_{jk} = \delta_{ik}$$

$$I = \begin{pmatrix} 1 & 0 & \dots \\ 0 & 1 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

$$I_{ij} = \delta_{ij} = \begin{cases} 1 & \text{for } i=j \\ 0 & \text{otherwise} \end{cases}$$

$$U_{ji}^* = \sum_j (\delta_{ij} + \Delta t K_{ji}^*)(\delta_{jk} + \Delta t K_{jk})$$

$$\approx \sum_j (\delta_{ij} \delta_{jk} + \Delta t \delta_{ij} K_{jk} + \Delta t \delta_{jk} K_{ji}^*) = \delta_{ik}$$

$$\delta_{ik} + \Delta t K_{ik} + \Delta t K_{ik}^* = \delta_{ik} + K_{ik}$$

$$\sum_j \delta_{ij} \delta_{jk} = \sum_{i \neq k} = \delta_{ik}$$

$\sum_j \delta_{ij} \delta_{ji} = \sum_j \delta_{ij}^2 = 1$ 
 $\sum_j \delta_{ij} \delta_{j2} =$

$\underbrace{K_{ik} + K_{ki}^*}_{K_{ik} = -\frac{i}{\hbar} H_{ik}} = 0$   
 $H_{ik} - H_{ki}^* = 0 \Rightarrow \hat{H} = \hat{H}^+$   
 $i\hat{L} = -i\hbar \hat{H}$

$$\hat{U}(\Delta t) = 1I - i/\hbar \hat{H} \Delta t$$

$\hat{U}$  Hamiltonka ali Hamiltonov operator

$$|\psi(t+\Delta t)\rangle = \hat{U} |\psi(t)\rangle = |\psi(t)\rangle - i/\hbar \Delta t \hat{H} |\psi(t)\rangle$$

$$i\hbar \frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t} = \hat{H} |\psi(t)\rangle$$

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

$$\hat{H} |i\rangle = \lambda_i |i\rangle$$

$$|\psi(t)\rangle = e^{-i\lambda_i t} |i\rangle$$

Schrödingerjeva enačba

$$|\psi(t=0)\rangle = |i\rangle$$

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

$$|\psi(t)\rangle = e^{-i\frac{\lambda_i}{\hbar}t}$$

$\omega_i$

$$i\hbar (-i\omega_i) e^{-i\omega_i t} |i\rangle = \lambda_i e^{-i\omega_i t} |i\rangle$$

$$\omega_i c = \lambda_i$$

$$\lambda_i < \hbar \omega_i = E_i$$

$\hat{H}$  je operator celotne energije sistema.  $\hat{H} = \hat{H}_{kin} + \hat{V}$

stacionarna stanja  $|\psi(t)\rangle = \underbrace{e^{-i\omega_i t}}_{\text{stano fazo se spreminja!}} |i\rangle$

Osnovna stanje  $|0\rangle$   $E_0 < E_1, E_2, E_3$

$\uparrow$   
vzdržljivo stanje  $|1\rangle, |2\rangle, \dots$

$$|\psi(t=0)\rangle = a|1\rangle + b|2\rangle$$

$$|\psi(t)\rangle = a e^{-i\omega_1 t}|1\rangle + b e^{-i\omega_2 t}|2\rangle$$

$$p_n(t) = |\langle 1 | \psi \rangle|^2 = |a|^2$$

$$a = b = 1/\sqrt{2}$$

Ali je sistem v stanju  $\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ ?

$$p_s(t) = |\langle s | \psi \rangle|^2$$

$$\langle s | \psi \rangle = \frac{1}{\sqrt{2}} (\langle 1 | + \langle 2 |) (a e^{-i\omega_1 t} |1\rangle + b e^{-i\omega_2 t} |2\rangle)$$

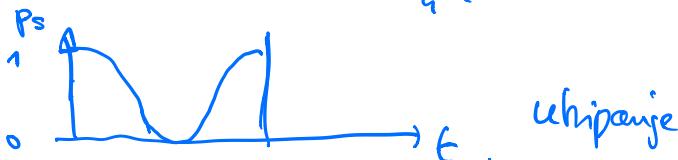
$$= \frac{1}{\sqrt{2}} (a e^{-i\omega_1 t} + b e^{-i\omega_2 t})$$

$$= \frac{1}{2} (e^{-i\omega_1 t} + e^{-i\omega_2 t})$$

$$p_s = \langle \psi | s \rangle \langle s | \psi \rangle = \frac{1}{4} (e^{-i\omega_1 t} + e^{-i\omega_2 t})(e^{i\omega_1 t} + e^{i\omega_2 t})$$

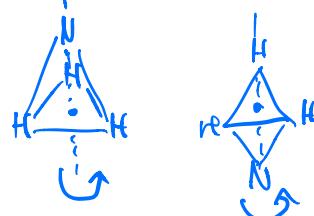
$$= \frac{1}{4} (1 + 1 + e^{i(\omega_1 - \omega_2)t} + e^{-i(\omega_1 - \omega_2)t})$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = |s\rangle = \frac{1}{4} (2 + 2 \cos(\omega_1 - \omega_2)t) = \frac{1 + \cos(\omega_1 - \omega_2)t}{2}$$



Amoniak

$NH_3$



$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi\rangle$$

$$|1\rangle$$

$$|2\rangle$$

$$|1\rangle, |2\rangle$$

$$|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle = \begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix} = \sum_{i=1}^2 c_i(t) |i\rangle$$

$$\langle i | i \hbar \frac{d}{dt} |\psi(t)\rangle = \langle i | \hat{H} |\psi\rangle$$

$$i\hbar \frac{d}{dt} \langle i | \psi(t)\rangle = \langle i | \hat{H} \hat{\psi}(t) | i \rangle$$

$$= \langle i | \hat{H} | \sum_j |j\rangle \langle j | \psi \rangle$$

$$\sum_j |j\rangle \langle j | = 1$$

$$i\hbar \dot{C}(t) = \sum_j \underbrace{\langle i | f(j) \rangle}_{H_{ij}} C_j(t)$$

$$i=1: \quad i\hbar \dot{C}_1 = H_{11} C_1 + H_{12} C_2$$

$$i=2: \quad i\hbar \dot{C}_2 = H_{22} C_2 + H_{21} C_1$$

$$H_{12} = H_{21} = 0 \quad i\hbar \dot{C}_1 = H_{11} C_1 \rightarrow C_1 = e^{-\frac{iH_{11}}{\hbar} t}$$

$$i\hbar \dot{C}_2 = H_{22} C_2 \rightarrow C_2 = e^{-\frac{iH_{22}}{\hbar} t}$$

$$H_{11} = H_{22} \approx E_0$$

$$H_{12} = H_{21}^* = -A \quad \text{fendrängung}$$

$$i\hbar \dot{C}_1 = E_0 C_1 - A C_2$$

$$i\hbar \dot{C}_2 = E_0 C_2 - A C_1$$

$$i\hbar \frac{d}{dt} (C_1 + C_2) = E_0 (C_1 + C_2) - A (C_1 + C_2)$$

$$C_1 + C_2 = \alpha e^{-\frac{i}{\hbar}(E_0 - A)t} \quad \leftarrow$$

$$i\hbar \frac{d}{dt} (C_1 - C_2) = E_0 (C_1 - C_2) + A (C_1 - C_2)$$

$$C_1 - C_2 = \beta e^{-i\hbar(E_0 + A)t} \quad \leftarrow$$

$$ZC_1 = \alpha e^{-i\hbar(E_0 - A)t} + \beta e^{-i\hbar(E_0 + A)t}$$

$$ZC_2 = \alpha e^{-i\hbar(E_0 - A)t} - \beta e^{-i\hbar(E_0 + A)t}$$

$$\begin{array}{llll} \alpha \neq 0 & \beta = 0 & C_1 = C_2 & E = E_0 - A \\ \alpha = 0 & \beta \neq 0 & C_1 = -C_2 & E = E_0 + A \end{array} \quad \text{razcep uivoja}$$